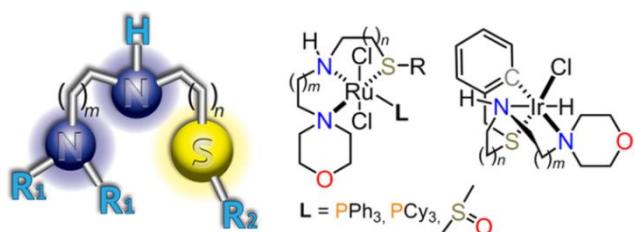


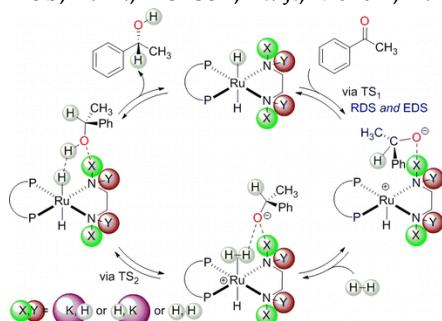
FULL LIST OF PUBLICATIONS

- * LANL (Apr 2013 – present):
- 7 (provisional pat. app.) **Macrocyclic ligands and their complexes for bifunctional molecular catalysis**
Dub, P. A.; Schmidt, J. G.; Gordon, J. C. Provisional Pat. Appl. US Serial No. 62/481,427 filed on April 4, 2017
- 6 (full paper) **Why does alkylation of the N–H functionality within M/NH bifunctional Noyori-type catalysts lead to turnover?**
Dub, P. A.; Scott, B. L.; Gordon, J. C. *J. Am. Chem. Soc.* **2017**, *139*(3), 1245.
- 5 (invited review) **The mechanism of enantioselective ketone reduction with Noyori and Noyori–Ikariya bifunctional catalysts.**
Dub, P. A.; Gordon, J. C. *Dalton Trans.* **2016**, *45*, 6756.
Selected as Cover Article.
- 4 (full paper) **First-row transition metal complexes of ENENES ligands: the ability of the thioether donor to impact the coordination chemistry.**
Dub, P. A.; Scott, B. L.; Gordon, J. C. *Dalton Trans.* **2016**, *45*, 1560.
- 3 (full paper) **Air-Stable NNS (ENENES) Ligands and their Well-Defined Ru and Ir Complexes for Molecular Catalysis.**
Dub, P. A.; Scott, B. L.; Gordon, J. C. *Organometallics* **2015**, *34*, 4464– 4479.



- 2 (patent) **POLYDENTATE LIGANDS AND THEIR COMPLEXES FOR MOLECULAR CATALYSIS.**
PCT Int. Appl. (2015), WO 2015191505 A1 20151217 (also appears as U.S. Pat. Appl. Publ. (2017), US 20170088571 A1 20170330)

- 1 (full paper) **Unravelling the Mechanism of the Asymmetric Hydrogenation of Acetophenone by [RuX₂(diphosphine)(1,2-diamine)] Catalysts.**
Dub, P. A.; Henson, N. J.; Martin, R. L.; Gordon, J. C. *J. Am. Chem. Soc.* **2014**, *136*, 3505–3521.



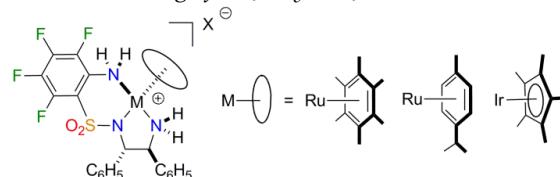
* From postdoctoral work at *Tokyo Institute of Technology* (Nov 2010 – Mar 2013):

⁷
(full paper) **Gram-Scale Hydrogenation of $\text{CF}_3\text{C(O)OCH}_3$ into $\text{CF}_3\text{CH(OH)OCH}_3$ or $\text{CF}_3\text{CH}_2\text{OH}$ With *trans*- $\text{RuH}_2(\text{CO})\text{dpa}$: Process, Key Intermediates, Catalytic Cycle and Origin of Chemoselectivity and Utmost Catalytic Performance.**

Dub, P. A.; Otsuka T.; Ishii A.; Ikariya, T. (*not submitted*)

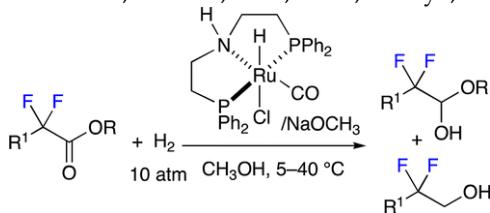
⁶
(full paper) **Ammonia as a Building Block to a Novel Class of Chiral Tridentate Ru and Ir Catalysts: via N–H Bond Activation Based on Metal–Ligand Cooperation and Mediated C–F Bond Cleavage.**

Dub, P. A.; Gridnev, I.; Kuwata, S.; Ikariya, T. *J. Am. Chem. Soc.* (*not submitted, presented at the 93rd Annual Meeting of CSJ, Kyoto, JAPAN, 22–25 March, 2013*)



⁵
(communication) **Practical Selective Hydrogenation of α -Fluorinated Esters with Bifunctional Pincer-Type Ruthenium(II) Catalysts Leading to Fluorinated Alcohols or Fluoral Hemiacetals.**

Otsuka T.; Ishii A.; Dub, P. A.; Ikariya, T. *J. Am. Chem. Soc.* **2013**, *135*, 9600–9603

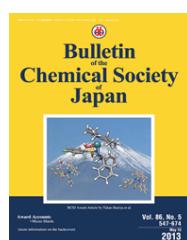
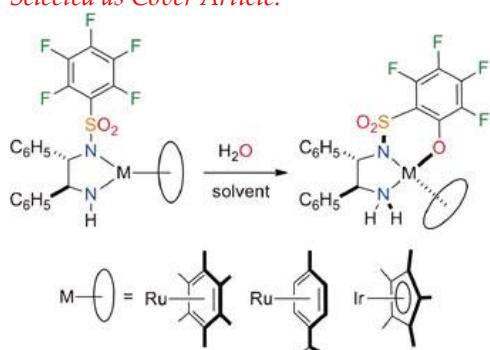


⁴
(full paper) **C–F Bond Breaking through Aromatic Nucleophilic Substitution with a Hydroxo Ligand Mediated via Water Bifunctional Activation.**

Dub, P. A.; Wang, H.; Matsunami, A.; Gridnev, I. D.; Kuwata, S.; Ikariya, T. *Bull. Chem. Soc. Jpn.* **2013**, *86*, 557–568.

*Bulletin of the Chemical Society of Japan Award Article, May 2013
(the most outstanding article among those that appear in each issue through selection by the Editorial Board), free pdf access.*

Selected as Cover Article.



 **BCSJ Award Article**
Bulletin of the Chemical Society of Japan
May 15, 2013

to

Pavel A. Dub

Department of Applied Chemistry, Graduate School of Science and Engineering,
Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152-8552

C–F Bond Breaking through Aromatic Nucleophilic Substitution with a Hydroxo Ligand Mediated via Water Bifunctional Activation
Pavel A. Dub, Hui Wang, Asuka Matsunami, Ilya D. Gridnev,
Shigeki Kuwata, and Takao Ikariya*
Bull. Chem. Soc. Jpn. **2013**, *86*, 557–568.

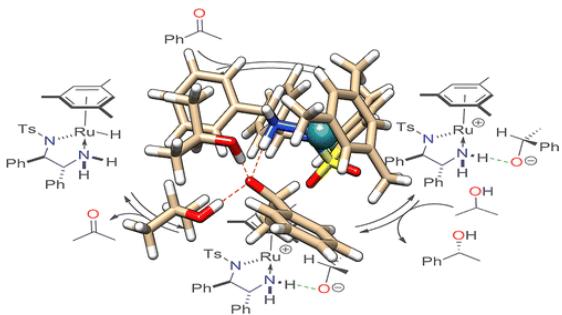
On behalf of the Chemical Society of Japan,
we certify that your article has been selected as the
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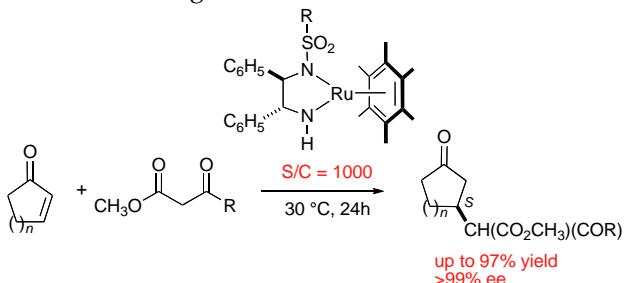
³
(full paper) **Quantum Chemical Calculations With the Inclusion of Nonspecific and Specific Solvation: Asymmetric Transfer Hydrogenation with Bifunctional Ruthenium Catalysts.**

Dub, P. A.; Ikariya, T. *J. Am. Chem. Soc.* **2013**, *135*, 2604–2619.



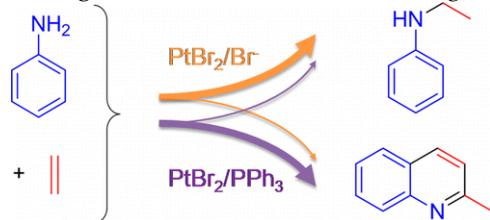
- ²
(invited
review) **Catalytic reductive transformations of carboxylic and carbonic acid derivatives using molecular hydrogen.**

- ¹ (communicati
on) **A Practical Asymmetric Conjugate Addition to Cyclic Enones with Chiral Bifunctional Ru Amido Catalysts.** Dub, P. A.; Wang, H.; Watanabe, M.; Gridnev, I.; Ikariya, T. *Tetrahedron Lett.* **2012**, *53*, 3452–3455.



[†] From graduate work at Laboratoire de Chimie de Coordination (UPR CNRS 8241):

- 10 (full paper) **Platinum-Catalyzed Assembly of Quinaldine from Aniline and Ethylene.**
Béthegnies, A.; Dub, P. A.; Poli, R. *Organometallics* 2013, 32, 1882–1891.



- ⁹ (full paper) Formation and Structure of a Platinum(II) Complex Containing Two trans Nonstabilized Phosphorus Ylide Ligands: Evidence for Reversible Ylide Dissociation.
Dub, P. A.; Béthegnies, A.; Daran, J.-C.; Poli, R. *Organometallics* **2012**, *31*, 3081–3086.

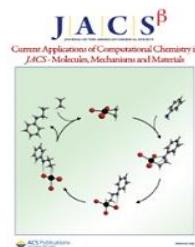
- 8 (full paper) **DFT and Experimental Studies on the PtX₂/X-Catalyzed Olefin Hydroamination: Effect of Halogen, Amine Basicity, and Olefin on Activity, Regioselectivity, and Catalyst Deactivation.**
Dub, P. A.; Béthegnies, A.; Poli, R. *Organometallics* **2012**, *31*, 294–305.

- ⁷ (full paper) Reactions of Diethylamine and Ethylene Catalyzed by PtII or Pt0 - Transalkylation vs. Hydroamination.
Dub, P. A.; Bethgnyes, A.; Poli, R., *Eur. J. Inorg. Chem.* **2011**, (33), 5167–5172.

- ⁶ Modeling the platinum-catalyzed intermolecular hydroamination of ethylene: the nucleophilic addition of HNEt₂ to coordinated ethylene in *trans*-PtBr₂(C₂H₄)(HNEt₂).
(invited full paper)

- ⁵ (full paper) **The Pt-catalyzed ethylene hydroamination by aniline: a computational investigation of the catalytic cycle.**

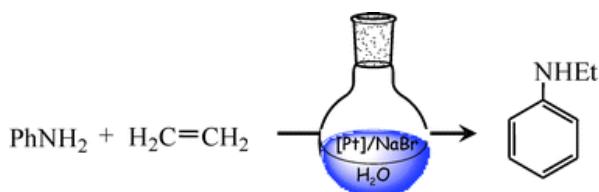
Dub, P. A.; Poli, R. *J. Am. Chem. Soc.* **2010**, *132* (39), 13799–13812.



JACS Select # 13, Ed. Prof. Weston T. Borden (2011) "Current Applications of Computational Chemistry in JACS – Molecules, Mechanisms and Materials". Selected as Cover Article.

- ⁴ (full paper) **Hydroamination of ethylene by aniline: catalysis in water.**

Dub, P. A.; R.-Zubiri, M.; Baudequin, C.; Poli, R. *Green Chem.* **2010**, *12*, 1392 – 1396.



- ³ (invited full paper) **A computational study of solution equilibria of platinum-based ethylene hydroamination catalytic species including solvation and counterion effects: Proper treatment of the free energy of solvation.**

Dub, P. A.; Poli, R. *J. Mol. Cat. A: Chem, Special issue on Computational Catalysis*, **2010**, *1-2*, 89–96.

- ² (full paper) **Experimental (IR, Raman) and computational analysis of a series of PtBr₂ derivatives: vibrational coupling in the coordinated ethylene and Pt-Br modes.**

Dub, P. A.; Filippov, O. A.; Belkova, N. V.; R.-Zubiri, M.; Poli, R. *J. Phys. Chem. A* **2009**, *113* (22), 6348–6355.

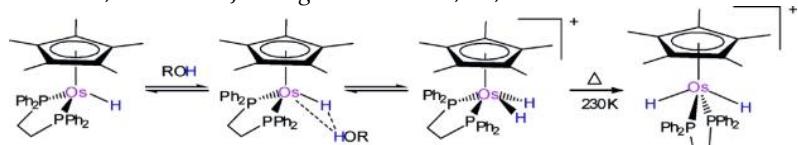
- ¹ (full paper) **The Pt-catalyzed ethylene hydroamination with aniline: synthesis, characterization and studies of intermediates.**

Dub, P. A.; R.-Zubiri, M.; Daran, J.-C.; Brunet, J.-J.; Poli, R. *Organometallics* **2009**, *28*, 4764–4777.

* From graduate work at A. N. Nesmeyanov Institute of Organoelement Compounds and student research work at HCC RAS:

- ¹⁰ (full paper) **Protonation of Cp*^{*}M(dppe)H hydrides: peculiarities of the osmium congener.**

Dub, P. A.; Filippov, O. A.; Silantyev, G. A.; Belkova, N. V.; Daran, J.-C.; Epstein, L. M.; Poli, R.; Shubina, E. S. *Eur. J. Inorg. Chem.* **2010**, *10*, 1489–1500.



- ⁹ (full paper) **Hydrogen bonding to carbonyl hydride complex Cp*^{*}Mo(PMe₃)₂(CO)H and its role in proton transfer.**

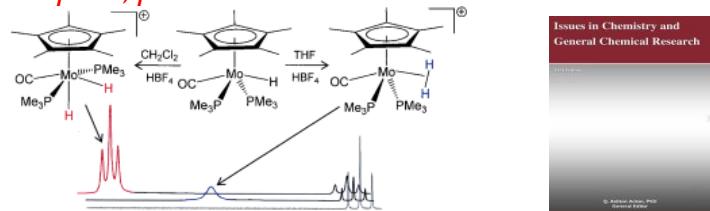
Dub, P. A.; Belkova, N. V.; Filippov, O. A.; Daran, J.-C.; Epstein, L. M.; Poli, R.; Shubina, E. S. *Dalton Trans.* **2010**, *39*, 2008–2015.

- ⁸ (full paper) **Solvent-Dependent Dihydrogen/Dihydride Stability for [Mo(CO)(Cp^{*})H₂(PMe₃)₂]⁺[BF₄]⁻ Determined by Multiple Solvent...Anion...Cation Non-Covalent Interactions.**

Dub, P. A.; Belkova, N. V.; Filippov, O. A.; Daran, J.-C.; Epstein, L. M.; Lledós, A.; Shubina, E. S.; Poli, R. *Chem. Eur. J.* **2010**, 16, 1, 189–201.

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Chapter 9, p. 2259.



7 **Investigation of the [Cp*Mo(PMe₃)₃H]ⁿ⁺ (*n* = 0, 1) redox pair: dynamic processes on very different timescales.**

Baya, M.; Dub, P. A.; Houghton, J.; Daran, J.-C.; Belkova, N. V.; Shubina, E. S.; Epstein, L. M.; Lledós, A.; Poli, R., *Inorg. Chem.* **2009**, 48, 209–220.

6 **Effect of the metal atom nature on hydrogen bonding and proton transfer to trihydride complexes Cp*MH₃(dppe): tungsten vs. molybdenum.**

Belkova, N. V.; Besora, M.; Baya, M.; Dub, P. A.; Epstein, L. M.; Lledós, A.; Poli, R., Revin, P. O.; Shubina, E. S. *Chem. Eur. J.* **2008**, 14, 9921–9934.

5 **Synthesis and Protonation Studies of Cp*Os(dppe)H: kinetics vs thermodynamics control.**

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4 **Solvent control in the protonation of Cp*Mo(dppe)H₃ by CF₃COOH.**

Dub, P. A.; Baya, M.; Houghton, J.; Belkova, N. V.; Daran, J.; Poli, R.; Epstein, L. M.; Shubina, E. S., *Eur. J. Inorg. Chem., special 10th anniversary issue*, **2007**, 2813–2826.

3 **Kinetics and Thermodynamics of Proton transfer to Cp*Ru(dppe)H: via dihydrogen bonding and (η²-H₂)-complex to the dihydride.**

Belkova, N. V.; Dub, P. A.; Baya, M.; Houghton, J. *Inorg. Chim. Acta, special issue "Inorganic Chemistry – The Next Generation"*, **2007**, 360, 149–162.

2 **Dihydrogen to Dihydride Isomerization Mechanism in [(C₅Me₅)FeH₂(Ph₂PCH₂CH₂PPh₂)]⁺ through the Experimental and Theoretical Analysis of Kinetic Isotope Effects.**

Baya, M.; Maresca, O.; Poli, R.; Coppel, Y.; Maseras, F.; Lledos, A.; Belkova, N. V.; Dub, P. A.; Epstein, L. M.; Shubina, E. S. *Inorg. Chem.* **2006**, 45, 10248v10262.

1 **Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to Cp*Fe(dppe)H.**

Belkova, N. V.; Collange, E.; Dub, P. A.; Epstein, L. M.; Lemenovskii, D. A.; Lledós, A.; Maresca, O.; Maseras, F.; Poli, R.; Revin, P. O.; Shubina, E. S.; Vorontsov, E. V. *Chem. Eur. J.* **2005**, 11, 873–888.